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 FILE LAST UPDATED: 21 Apr 2009 (20090421/ED)

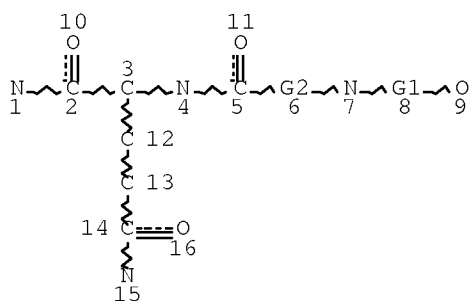
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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que l4
 L1 STR



REP G1=(1-2) C
 REP G2=(10-10) C
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
 L3 22 SEA FILE=REGISTRY SSS FUL L1

L4 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d ibib abs hitstr l4 1-12

L4 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1284828 HCAPLUS Full-text

DOCUMENT NUMBER: 148:130122

TITLE: Templated polypyrrole electro-polymerization:
Self-assembled bundles of bilayer membranes of
amphiphiles and their actuation behaviorAUTHOR(S): Kagawa, Kazuhiro; Qian, Pu; Tanaka, Akihisa; Swager,
Timothy M.CORPORATE SOURCE: Fundamental Technology Research Center, Honda R&D Co.
Ltd., 1-4-1 Chuo Wako-shi, Saitama, 351-0193, Japan

SOURCE: Synthetic Metals (2007), 157(18-20), 733-738

CODEN: SYMEDZ; ISSN: 0379-6779

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electrochem. properties of conducting polymers are highly dependent on the microstructure. The authors report a method to produce specific microstructures of polypyrrole through electropolymn. in the presence of the amphiphile N-{11-(2-hydroxyethyl)dimethylammonium}undecanoyl}-N,N'- dioctyl-L-glutamate, bromide, which forms supramol. hydrogels with pyrrole in aqueous solution. These hydrogels were used as templates during polypyrrole electropolymn. to give microstructures composed of the bundles of bilayer membranes. The highly porous nature of these films resulted in electrochem. properties superior to polypyrrole deposited under the same condition without use of an amphiphilic template. Anal. of the scan rate dependence on cyclic voltammogram reveals that the porous templated films facilitate fast diffusion of dopant ions. The actuation properties were also studied in aqueous solns. containing Na p-toluenesulfonate electrolyte. The strains displayed by the template polypyrrole films were twice those synthesized without the use of a template.

IT 479671-12-0

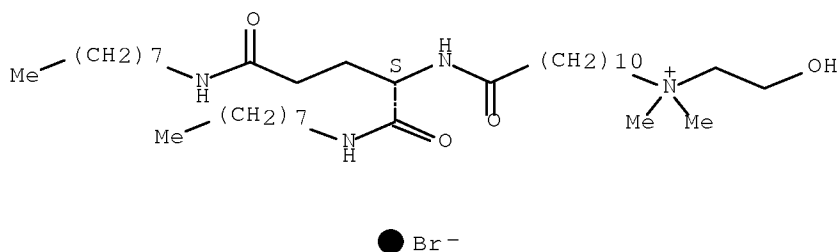
RL: NUU (Other use, unclassified); USES (Uses)

(templated electropolymn. of pyrrole on ITO from Na toluenesulfonate using amphiphile ammonium glutamic acid amide assembled into supramol. hydrogels giving polypyrrole with higher strain in actuator applications)

RN 479671-12-0 HCAPLUS

CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-(octylamino)-1-[(octylamino)carbonyl]-4-oxobutyl]amino]-11-oxo-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

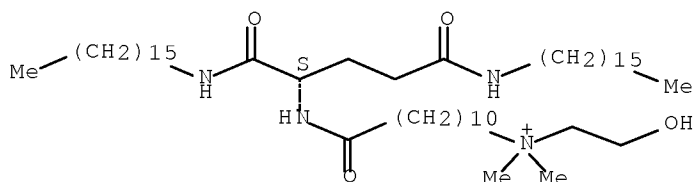
L4 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2007:280690 HCAPLUS Full-text
 DOCUMENT NUMBER: 146:317787
 TITLE: Self-assembling inorganic nanoparticle-organic compound composites, cured resins containing them, and their manufacture
 INVENTOR(S): Narikiyo, Yoshitaka; Ogami, Shinya; Kimizuka, Nobuo
 PATENT ASSIGNEE(S): Kyoritsu Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 20pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2007063232	A	20070315	JP 2005-254647	20050902
PRIORITY APPLN. INFO.:			JP 2005-254647	20050902
OTHER SOURCE(S):	MARPAT 146:317787			

AB The invention relates to composites comprising inorg. nanoparticles and self-assembling organic compds. Thus, mixing a toluene solution of N-(11-dimethylhydroxyethylammoniumundecanoyl)-L-glutamic acid dihexadecyldiamide with an aqueous solution of H₂AuCl₄, heating at 120°, and reducing the metal salt gave a toluene solution of composite Au nanoparticles showing nanowire structure and reversible sol-gel transformation.

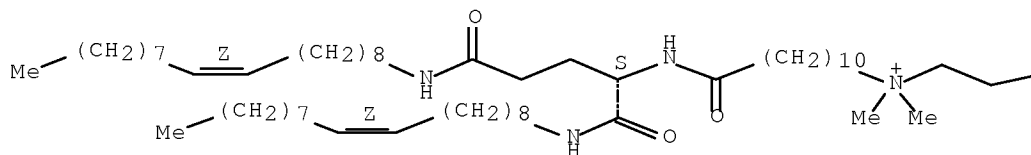
IT 763925-94-6P 928707-56-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (self-assembling inorg. nanoparticle-organic compound composites)
 RN 763925-94-6 HCAPLUS
 CN 1-Undecanaminium, 11-[[[(1S)-4-(hexadecylamino)-1-[(hexadecylamino)carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo- (CA INDEX NAME)]

Absolute stereochemistry.



RN 928707-56-6 HCAPLUS
 CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-[(9Z)-9-octadecen-1-ylamino]-1-[[[(9Z)-9-octadecen-1-ylamino]carbonyl]-4-oxobutyl]amino]-11-oxo- (CA INDEX NAME)]

Absolute stereochemistry.
 Double bond geometry as shown.



—OH

L4 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:1031055 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 142:276104
 TITLE: Gastrin receptor-avid peptide conjugates
 INVENTOR(S): Higginbotham, Chrys-Ann; Sieckman, Gary; Hoffman, Timothy J.; Volkert, Wynn A.; Li, Ning
 PATENT ASSIGNEE(S): University of Missouri, USA
 SOURCE: Can. Pat. Appl., 117 pp.
 CODEN: CPXXEB
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2346154	A1	20021102	CA 2001-2346154	20010502
PRIORITY APPLN. INFO.:			CA 2001-2346154	20010502

AB A compound for use as a therapeutic or diagnostic radiopharmaceutical includes a group capable of complexing a medically useful metal attached to a moiety which is capable of binding to a gastrin releasing peptide receptor. A method for treating a subject having a neoplastic disease includes administering to the subject an effective amount of a radiopharmaceutical having a metal chelated with a chelating group attached to a moiety capable of binding to a gastrin releasing peptide receptor expressed on tumor cells with subsequent internalization inside of the cell. A method of forming a therapeutic or diagnostic compound includes reacting a metal synthon with a chelating group covalently linked with a moiety capable of binding a gastrin releasing peptide receptor.

IT 422512-84-3

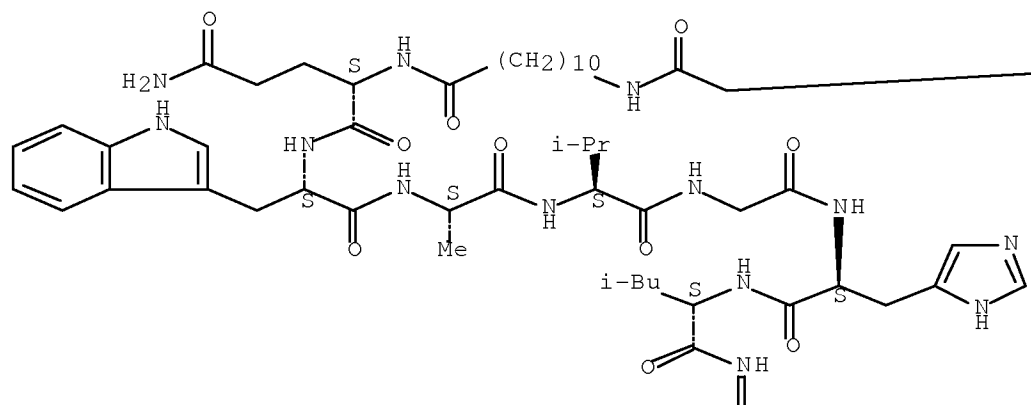
RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (gastrin receptor-avid peptide conjugates)

RN 422512-84-3 HCAPLUS

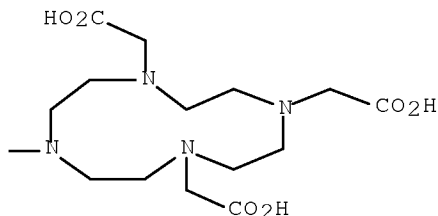
CN L-Methioninamide, N2-[1-oxo-11-[[[4,7,10-tris(carboxymethyl)-1,4,7,10-tetraazacyclododec-1-yl]acetyl]amino]undecyl]-L-glutaminy-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

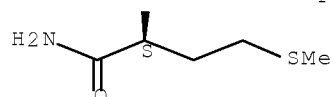
PAGE 1-A



PAGE 1-B



PAGE 2-A



L4 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:249522 HCAPLUS Full-text
 DOCUMENT NUMBER: 140:287105
 TITLE: Preparation of organic-inorganic nanoparticle
 composites and their components for one-dimensionally
 assembled structures and gels with organic solvents
 INVENTOR(S): Kimizuka, Nobuo; Matsune, Hideki; Ogami, Shinya
 PATENT ASSIGNEE(S): Kyoritsu Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004091328	A	20040325	JP 2002-250830	20020829
PRIORITY APPLN. INFO.:			JP 2002-250830	20020829

OTHER SOURCE(S): MARPAT 140:287105

AB The composites, preferably forming one-directional alignments or their crosslinked structures spontaneously, or gelling organic solvents, are prepared by mixing organic compound-protected inorg. nanoparticles with amphiphilic organic compds. in polar solvents, followed by removing the solvents. Thus, H₂AuCl₄ was dissolved with [4-HOC₆H₄CONH(CH₂)₂S]₂ (I) in MeOH and reduced with NaBH₄ to give I-protected Au nanoparticles, which were mixing with Me(CH₂)₁₅NHCOCH[(CH₂)₂CONH(CH₂)₁₅Me]NHCO(CH₂)₁₀N+Me₂CH₂CH₂OHBr⁻ on MeOH, and MeOH was evaporated to give a composite. The composite was dissolved in chlorocyclohexane at 100° and cooled to room. temperature to give a gel containing interlaced network comprising one-directional alignment of the composite.

IT 215612-51-4 675603-09-5 675603-10-8

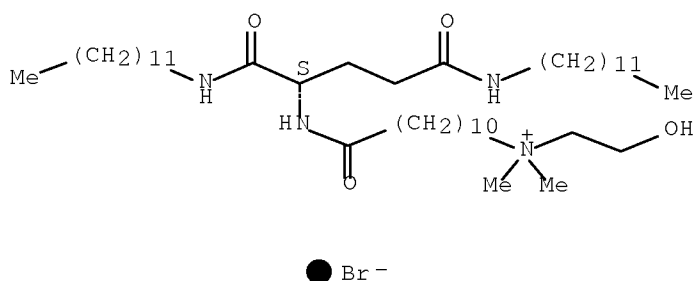
RL: MSC (Miscellaneous)

(preparation of organic compound-protected inorg. nanoparticle-amphiphilic organic compound composites for one-dimensionally assembled structures and gels with organic solvents)

RN 215612-51-4 HCAPLUS

CN 1-Undecanaminium, 11-[[[(1S)-4-(dodecylamino)-1-[(dodecylamino)carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo-, bromide (1:1)
(CA INDEX NAME)

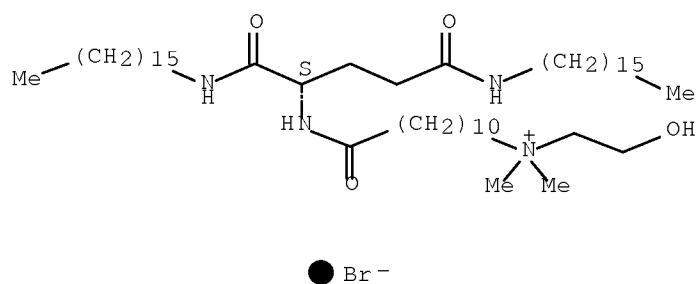
Absolute stereochemistry.



RN 675603-09-5 HCAPLUS

CN 1-Undecanaminium, 11-[[[(1S)-4-(hexadecylamino)-1-[(hexadecylamino)carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo-, bromide (1:1) (CA INDEX NAME)

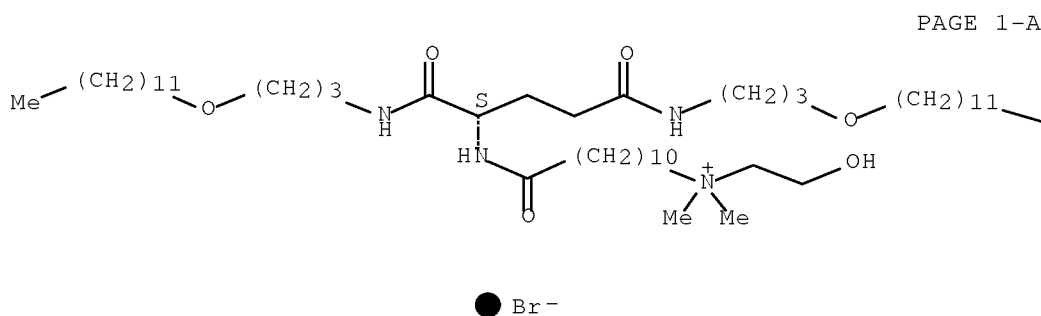
Absolute stereochemistry.



RN 675603-10-8 HCAPLUS

CN 1-Undecanaminium, 11-[[[(1S)-4-[[3-(dodecyloxy)propyl]amino]-1-[[[3-(dodecyloxy)propyl]amino]carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-B

Me

IT 675603-08-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of organic compound-protected inorg. nanoparticle-amphiphilic organic

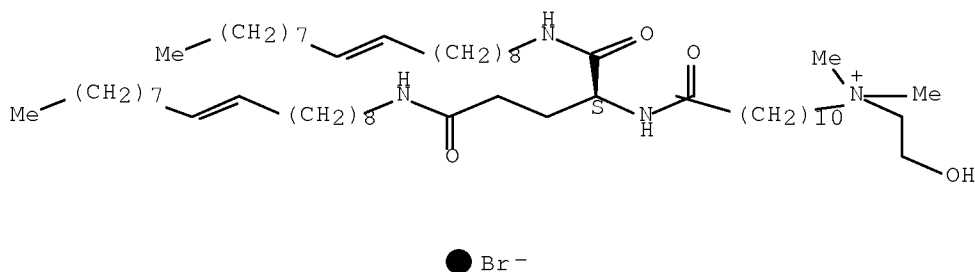
compound composites for one-dimensionally assembled structures and gels with organic solvents)

RN 675603-08-4 HCAPLUS

CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-(9-octadecen-1-ylamino)-1-[(9-octadecen-1-ylamino)carbonyl]-4-oxobutyl]amino]-11-oxo-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



L4 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:143197 HCAPLUS Full-text
 DOCUMENT NUMBER: 140:165218
 TITLE: Molecule alignment polymer gel and molecule alignment polymer cast film having self-organizing amphiphilic compound as template and process for producing the same
 INVENTOR(S): Kimizuka, Nobuo; Kagawa, Kazuhiro; Nakashima, Takuya
 PATENT ASSIGNEE(S): Honda Giken Kogyo Kabushiki Kaisha, Japan
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014965	A1	20040219	WO 2003-JP10068	20030807
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003254862	A1	20040225	AU 2003-254862	20030807
EP 1553109	A1	20050713	EP 2003-784575	20030807
EP 1553109	B1	20071024		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
US 20060102876	A1	20060518	US 2005-524079	20051031
PRIORITY APPLN. INFO.:			JP 2002-231958	A 20020808
			JP 2003-13943	A 20030122
			WO 2003-JP10068	W 20030807

AB The invention relates to a mol. alignment polymer gel and a mol. alignment polymer film produced by the self-organization of a self-organizing amphiphilic compound with a monomer interacting with this amphiphilic compound followed by the polymerization of the monomer; and a process for producing the same.

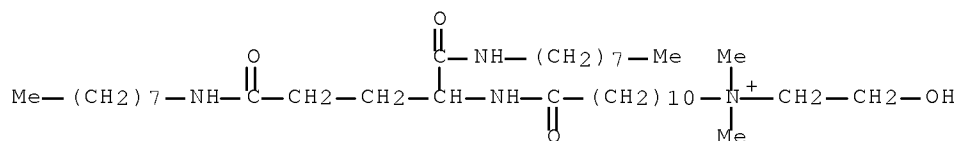
IT ~~656837-99-9~~ 656838-00-5

RL: NUU (Other use, unclassified); USES (Uses)

(template; mol. alignment polymer gel and mol. alignment polymer cast film having self-organizing amphiphilic compound as template and process for producing the same)

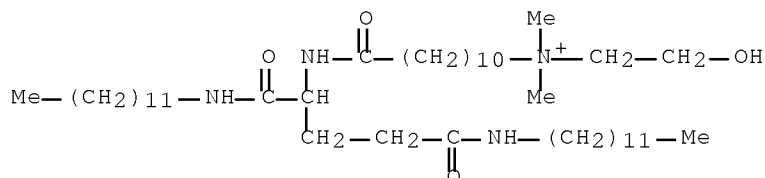
RN 656837-99-9 HCAPLUS

CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[4-(octylamino)-1-[(octylamino)carbonyl]-4-oxobutyl]amino]-11-oxo- (CA INDEX NAME)



RN 656838-00-5 HCAPLUS

CN 1-Undecanaminium, 11-[[4-(dodecylamino)-1-[(dodecylamino)carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:509850 HCAPLUS Full-text

DOCUMENT NUMBER: 140:141967

TITLE: A new lipophilic fluorescent probe for interaction studies of bioactive lipopeptides with membrane models
AUTHOR(S): Peroni, Elisa; Caminati, Gabriella; Baglioni, Piero; Chelli, Mario; Papini, Anna M.

CORPORATE SOURCE: Dipartimento di Chimica, Universita degli Studi di Firenze, Florence, I-50121, Italy

SOURCE: Peptides 2000, Proceedings of the European Peptide Symposium, 26th, Montpellier, France, Sept. 10-15, 2000 (2001), Meeting Date 2000, 989-990. Editor(s): Martinez, Jean; Fehrentz, Jean-Alain. Editions EDK: Paris, Fr.

CODEN: 69EDWK; ISBN: 2-84254-048-4

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Lipophilic fluorescent probes with alkyl chains of different lengths were synthesized as building-blocks to obtain fluorescent labeled mols. Peptides with a lipophilic moiety at the N-terminus interact with much more affinity with the membrane compared to the lipid free analogs due to their permanence in the cell membrane and to a subsequent facilitated interaction with membrane receptors.

IT 457904-58-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

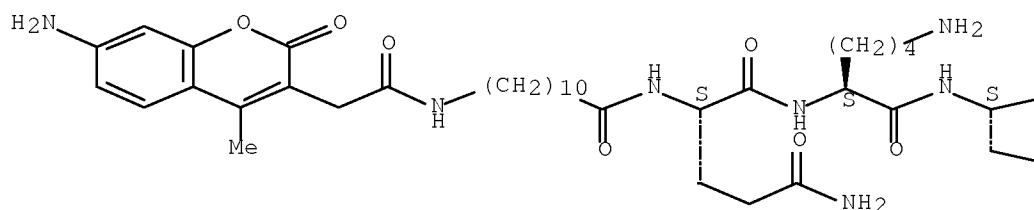
(lipophilic fluorescent probe for interaction studies of bioactive
lipopeptides with membrane models)

RN 457904-58-4 HCAPLUS

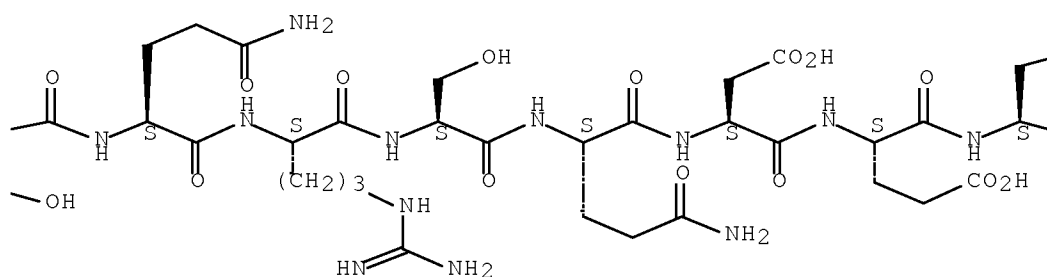
CN L-Valinamide, N2-[11-[[[(7-amino-4-methyl-2-oxo-2H-1-benzopyran-3-yl)acetyl]amino]-1-oxoundecyl]-L-glutaminy-L-lysyl-L-seryl-L-glutaminy-L-arginyl-L-seryl-L-glutaminy-L- α -aspartyl-L- α -glutamyl-L-asparaginy-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

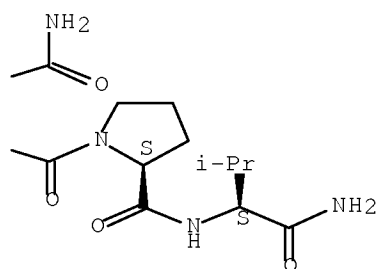
PAGE 1-A



PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:426139 HCAPLUS Full-text

DOCUMENT NUMBER: 140:73229

TITLE: Novel series of ¹¹¹In-labeled bombesin analogs as potential radiopharmaceuticals for specific targeting of gastrin-releasing peptide receptors expressed on human prostate cancer cells

AUTHOR(S): Hoffman, Timothy J.; Gali, Hariprasad; Smith, C. Jeffrey; Sieckman, Gary L.; Hayes, Donald L.; Owen, Nellie K.; Volkert, Wynn A.

CORPORATE SOURCE: Research Service, Harry S. Truman Memorial VA Hospital, Columbia, MO, USA

SOURCE: Journal of Nuclear Medicine (2003), 44(5), 823-831
CODEN: JNMEAQ; ISSN: 0161-5505

PUBLISHER: Society of Nuclear Medicine

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Gastrin-releasing peptide (GRP) receptors have been shown to be expressed with high densities on several types of cancer cells including prostate, breast, small cell lung, and pancreas cancers. Bombesin (BBN) has been known to bind to GRP receptors with high affinity and specificity. The aim of these studies was to develop new ¹¹¹In-labeled BBN analogs having high tumor uptake and optimal pharmacokinetics for specific targeting of human prostate cancers. Methods: A novel series of dodecanetetraacetic acid (DOTA)-X-BBN[7-14]NH₂ (X = 0, β -Ala, 5-Ava, 8-Aoc, or 11-Aun) conjugates and their In(III)/¹¹¹In complexes exhibiting high GRP-receptor-binding affinities were synthesized and characterized. Results: In vitro competitive binding assays, using PC-3 androgen-independent human prostate cancer cells, demonstrated values of <2.5 nmol/L for inhibitory concentration of 50% for analogs with β -Ala, 5-Ava, and 8-Aoc spacers. In vivo biodistribution studies of the ¹¹¹In-DOTA-X-BBN[7-14]NH₂ conjugates performed on CF-1 mice at 1 h after injection have revealed that the uptake of radioactivity in the pancreas, a GRP-receptor-expressing tissue, increased as a function of hydrocarbon spacer length (i.e., from 0.20 \pm 0.04 percentage injected dose [%ID] per g for the analog with no spacer to a maximum of 26.97 \pm 3.97 %ID/g for the analog with 8-Aoc spacer). The radioactivity was cleared efficiently from the blood pool by excretion mainly through the renal/urinary pathway (e.g., 71.6 \pm 1.8 %ID at 1 h after injection for 8-Aoc spacer analog). In vivo pharmacokinetic studies of the ¹¹¹In-DOTA-8-Aoc-BBN[7-14]NH₂ conjugate conducted on PC-3 human prostate cancer-derived xenografts in SCID mice showed a specific uptake of radioactivity in tumor, with 3.63 \pm 1.11 %ID/g observed at 1 h after injection. High tumor-to-blood and tumor-to-muscle ratios of approx. 6:1 and 45:1, resp., were achieved at 1 h after injection. Relative to the radioactivity observed in the tumor at 1 h after injection, 43%, 19%, and 9% of the radioactivity was retained at, resp., 24, 48, and 72 h after injection. Conclusion: These studies showed that radiometallated DOTA-X-BBN[7-14]NH₂ constructs with hydrocarbon spacers ranging from 5 to 8 carbon atoms are feasible candidates for further development as diagnostic and therapeutic radiopharmaceuticals for patients with GRP-pos. cancers.

IT 422512-84-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(¹¹¹In-labeled bombesin analogs as potential radiopharmaceuticals for

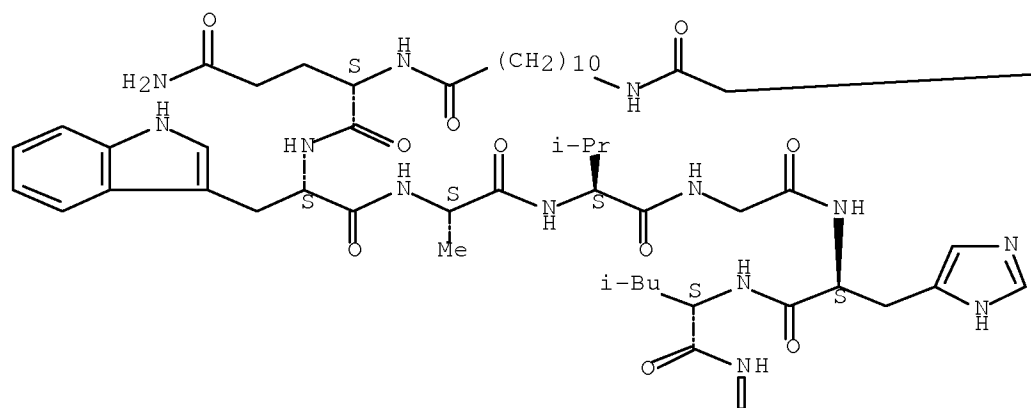
specific targeting of gastrin-releasing peptide receptors expressed on human prostate cancer cells)

RN 422512-84-3 HCAPLUS

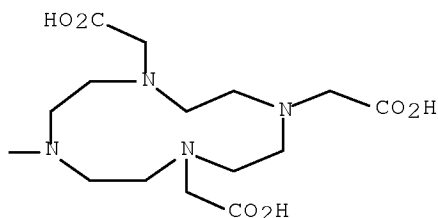
CN L-Methioninamide, N2-[1-oxo-11-[[[4,7,10-tris(carboxymethyl)-1,4,7,10-tetraazacyclododec-1-yl]acetyl]amino]undecyl]-L-glutamyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

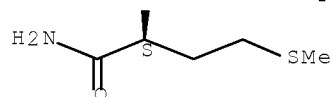
PAGE 1-A



PAGE 1-B



PAGE 2-A



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:951548 HCAPLUS Full-text

DOCUMENT NUMBER: 138:149623
 TITLE: Radiochemical Investigations of
 99mTc-N3S-X-BBN[7-14]NH₂: An in Vitro/in Vivo
 Structure-Activity Relationship Study Where X = 0-,
 3-, 5-, 8-, and 11-Carbon Tethering Moieties
 AUTHOR(S): Smith, C. Jeffrey; Gali, Hariprasad; Sieckman, Gary
 L.; Higginbotham, Chris; Volkert, Wynn A.; Hoffman,
 Timothy J.
 CORPORATE SOURCE: Research Services, Harry S. Truman Memorial Veterans'
 Hospital, Columbia, MO, 65201, USA
 SOURCE: Bioconjugate Chemistry (2003), 14(1), 93-102
 CODEN: BCCHE; ISSN: 1043-1802
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Bombesin (BBN), a 14 amino acid peptide, is an analog of human gastrin releasing peptide (GRP) that binds to GRP receptors (GRPr) with high affinity and specificity. The GRPr is overexpressed on a variety of human cancer cells, including prostate, breast, lung, and pancreatic cancers. The specific aim of this study was to develop 99mTc-radiolabeled BBN analogs that maintain high specificity for the GRPr in vivo. A preselected synthetic sequence via solid-phase peptide synthesis (SPPS) was designed to produce N3S-BBN (N3S = dimethylglycyl-L-seryl-L-cysteinylglycinamide) conjugates with the following general structure: DMG-S-C-G-X-Q-W-A-V-G-H-L-M-(NH₂), where the spacer group, X = 0 (no spacer), ω-NH₂(CH₂)₂COOH, ω-NH₂(CH₂)₄COOH, ω-NH₂(CH₂)₇COOH, or ω-NH₂-(CH₂)₁₀COOH. The new BBN constructs were purified by reversed phase-HPLC (RP-HPLC). Electrospray mass spectrometry (ES-MS) was used to characterize the nonmetalated BBN conjugates. Re(V)-BBN conjugates were prepared by the reaction of Re(V)gluconate with N3S-X-BBN[7-14]NH₂ (X = 0 carbons, β-Ala (β-alanine), 5-Ava (5-aminovaleric acid), 8-Aoc (8-aminooctanoic acid), and 11-Aun (11-aminoundecanoic acid)) with gentle heating. Re-N3S-5-Ava-BBN[7-14]NH₂ was also prepared by the reaction of [Re(V)dimethylglycyl-L-seryl-L-cysteinylglycinamide] with 5-Ava-BBN[7-14]NH₂. ES-MS was used to determine the mol. constitution of the new Re(V) conjugates. The 99mTc conjugates were prepared at the tracer level by each the prelabeling, post-conjugation and pre-conjugation, postlabeling approaches from the reaction of Na[99mTcO₄] with excess SnCl₂, sodium gluconate, and corresponding ligand. The 99mTc and Re(V) conjugates behaved similarly under identical RP-HPLC conditions. In vitro and in vivo models demonstrated biol. integrity of the new conjugates.

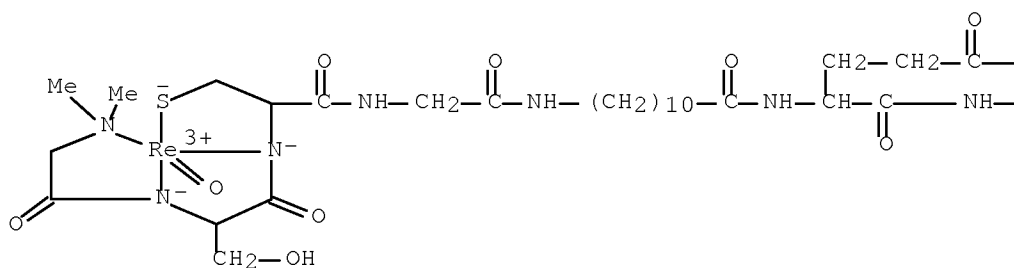
IT ~~496034-07-2P~~ 496034-80-1P

RL: DGN (Diagnostic use); PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 99mTc-radiolabeled bombesin analogs with high specificity for gastrin releasing peptide receptors)

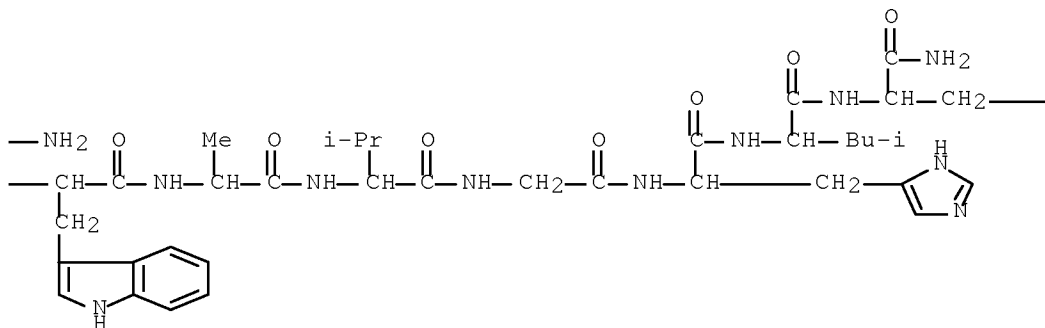
RN 496034-07-2 HCAPLUS

CN Rhenium, [N,N-dimethylglycyl-κN-L-seryl-κN-L-cysteinyl-κN,κS-glycyl-11-aminoundecanoyl-L-glutaminyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl-L-methioninamidato(3-)]oxo-, (SP-5-25)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

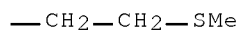
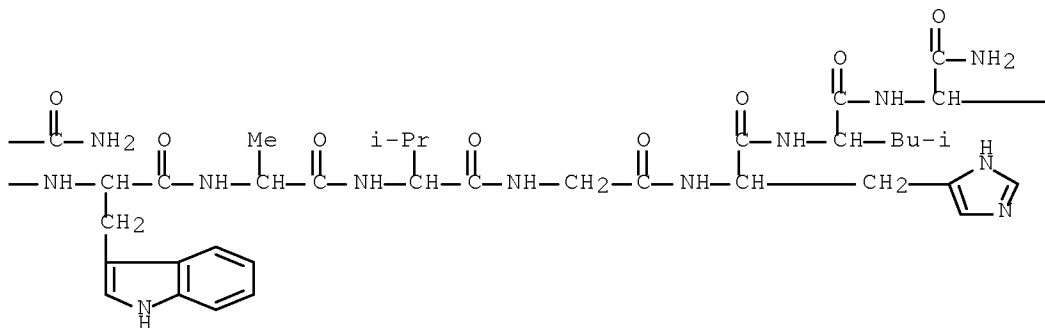
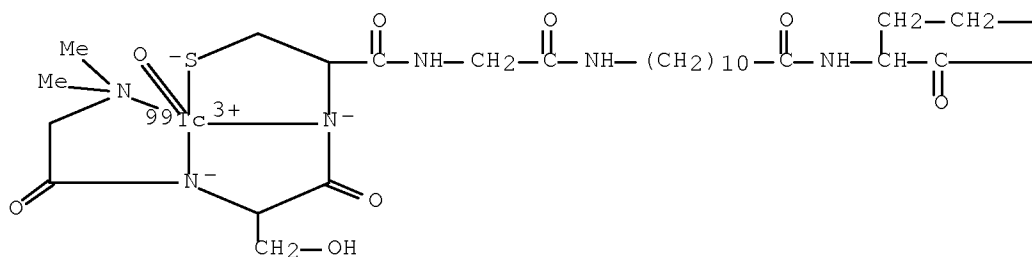


PAGE 1-C

—CH₂—SMe

RN 496034-80-1 HCAPLUS

CN Technetium-99Tc, [N,N-dimethylglycyl-κN-L-seryl-κN-L-cysteinyl-
 κN,κS-glycyl-11-aminoundecanoyl-L-glutamyl-L-tryptophyl-L-
 alanyl-L-valylglycyl-L-histidyl-L-leucyl-L-methioninamidato(3-)]-,
 (SP-5-25)- (9CI) (CA INDEX NAME)



IT 495391-17-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

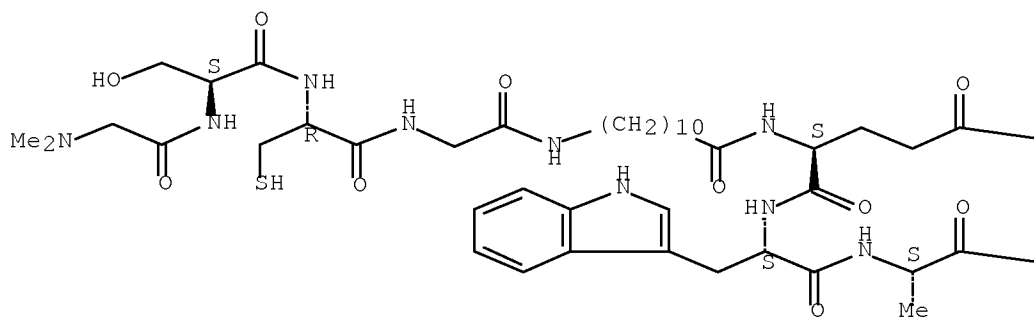
(preparation of ^{99m}Tc -radiolabeled bombesin analogs with high specificity for gastrin releasing peptide receptors)

RN 495391-17-8 HCAPLUS

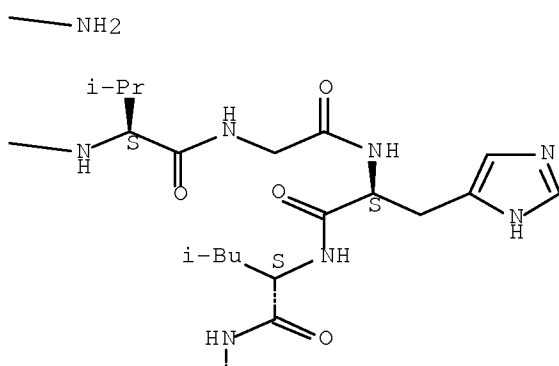
CN	L-Methioninamide, N,N-dimethylglycyl-L-seryl-L-cysteinylglycyl-11-aminoundecanoyl-L-glutaminy-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

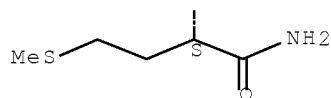
PAGE 1-A



PAGE 1-B



PAGE 2-B



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:658880 HCAPLUS [Full-text](#)

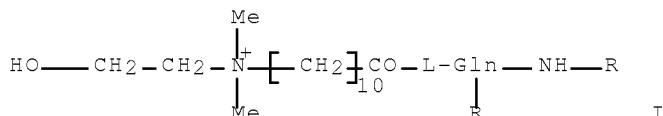
DOCUMENT NUMBER: 138:73478

TITLE: Light-harvesting supramolecular hydrogels assembled from short-legged cationic L-glutamate derivatives and anionic fluorophores

AUTHOR(S): Nakashima, Takuya; Kimizuka, Nobuo

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Graduate

SOURCE: School of Engineering, Kyushu University, Fukuoka,
812-8581, Japan
Advanced Materials (Weinheim, Germany) (2002), 14(16),
1113-1116
CODEN: ADVMEW; ISSN: 0935-9648
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:73478
GI



AB Cationic L-glutamate derivs. [I; R = (CH₂)₇, CH(CH₃)₂] were prepared from I [R = (CH₂)₁₁CH₃] for use as self-assembling receptors of fluorescent compds. 2-naphthalene sulfonate or 9,10-dimethoxy-2-anthracene sulfonate. Aqueous dispersions of I were prepared by ultrasonification, and found to show self-assembly behavior. Addition of fluorescent agents to I (R = (CH₂)₇, CH(CH₃)₂) gave hydrogels whose fluorescent properties were investigated as light-harvesting supramol. networks.

IT 479671-15-3P 479671-17-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescent behavior of as light-harvesting supramol. hydrogels)

RN 479671-15-3 HCAPLUS

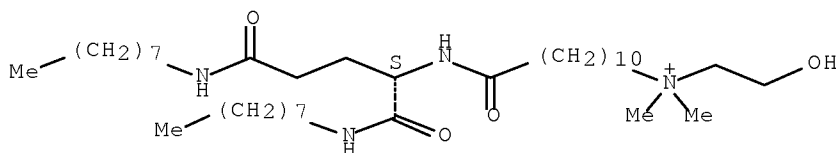
CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-(octylamino)-1-[(octylamino)carbonyl]-4-oxobutyl]amino]-11-oxo-, 2-naphthalenesulfonate (1:1) (CA INDEX NAME)

CM 1

CRN 479671-14-2

CMF C36 H73 N4 O4

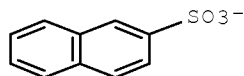
Absolute stereochemistry.



CM 2

CRN 16023-36-2

CMF C10 H7 O3 S



RN 479671-17-5 HCAPLUS

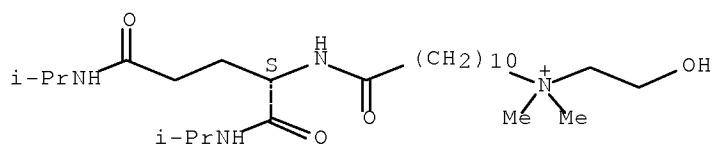
CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-[(1-methylethyl)amino]-1-[[[(1-methylethyl)amino]carbonyl]-4-oxobutyl]amino]-11-oxo-, salt with 9,10-dimethoxy-2-anthracenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 479671-16-4

CMF C26 H53 N4 O4

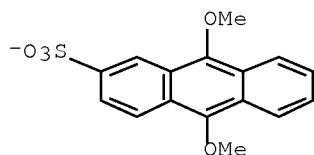
Absolute stereochemistry.



CM 2

CRN 137308-85-1

CMF C16 H13 O5 S



IT 479671-12-0P 479671-13-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

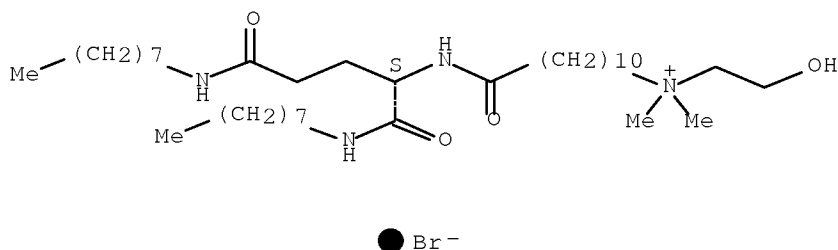
(preparation and reaction of in the preparation of light-harvesting supramol.

hydrogels using cationic L-glutamate derivs. and anionic fluorophores)

RN 479671-12-0 HCAPLUS

CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-(octylamino)-1-[(octylamino)carbonyl]-4-oxobutyl]amino]-11-oxo-, bromide (1:1) (CA INDEX NAME)

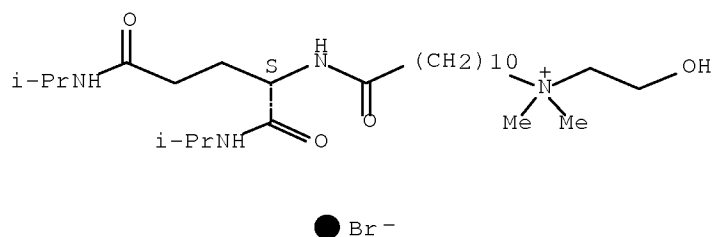
Absolute stereochemistry.



RN 479671-13-1 HCAPLUS

CN 1-Undecanaminium, N-(2-hydroxyethyl)-N,N-dimethyl-11-[[[(1S)-4-[(1-methylethyl)amino]-1-[[[(1-methylethyl)amino]carbonyl]-4-oxobutyl]amino]-11-oxo-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



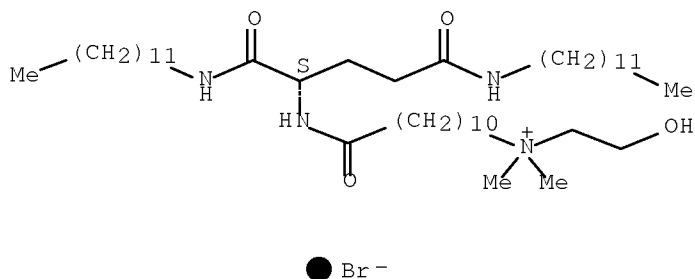
IT 215612-51-4

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(reaction of in the preparation of light-harvesting supramol. hydrogels
using cationic L-glutamate derivs. and anionic fluorophores)

RN 215612-51-4 HCAPLUS

CN 1-Undecanaminium, 11-[[[(1S)-4-(dodecylamino)-1-[(dodecylamino)carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo-, bromide (1:1)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:438603 HCAPLUS Full-text

DOCUMENT NUMBER: 137:275171
 TITLE: A new lipophilic fluorescent probe for interaction studies of bioactive lipopeptides with membrane models
 AUTHOR(S): Peroni, Elisa; Caminati, Gabriella; Baglioni, Piero; Nuti, Francesca; Chelli, Mario; Papini, Anna M.
 CORPORATE SOURCE: Polo Scientifico, Dipartimento di Chimica Organica 'Ugo Schiff', Universita degli Studi di Firenze, (FI), Sesto Fiorentino, I-50019, Italy
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(13), 1731-1734
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

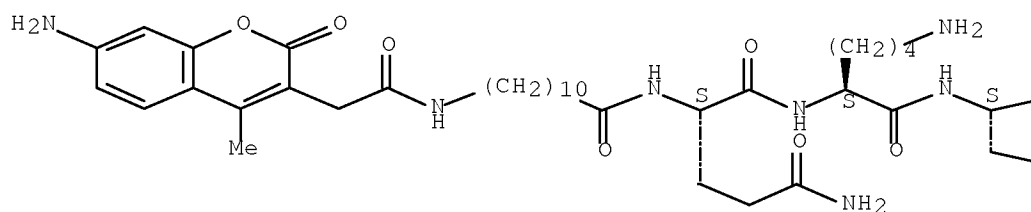
AB The new fluorescent lipophilic moiety 11-[(7-amino-4-methyl-2-oxo-2H-1-benzopyran-3-acetyl)amino]undecanoic acid (AMCA-~~ω~~Aud-OH) was introduced by SPPS at the N-terminus of the immunodominant epitope GpMBP(74-85). FRET expts. using the new fluorescent lipopeptide demonstrate that the peptide interacts with much more affinity with the membrane compared to the lipid free analog.

IT 457904-58-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (new lipophilic fluorescent probe for interaction studies of bioactive lipopeptides with membrane models)

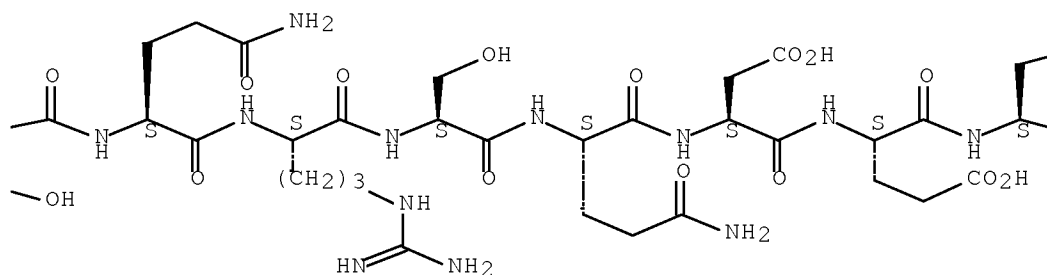
RN 457904-58-4 HCAPLUS
 CN L-Valinamide, N2-[11-[[[(7-amino-4-methyl-2-oxo-2H-1-benzopyran-3-yl)acetyl]amino]-1-oxoundecyl]-L-glutaminyL-L-lysyl-L-seryl-L-glutaminyL-L-arginyl-L-seryl-L-glutaminyL-L- α -aspartyl-L- α -glutamyl-L-asparaginyL-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

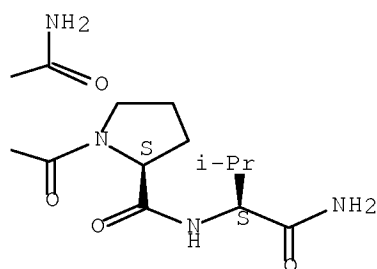
PAGE 1-A



PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:353971 HCAPLUS Full-text

DOCUMENT NUMBER: 136:365879

TITLE: Gastrin receptor-avid peptide conjugates and radionuclide complexes

INVENTOR(S): Hoffman, Timothy J.; Volkert, Wynn A.; Sieckman, Gary; Smith, Charles J.; Gali, Hariprasad

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 60 pp., Cont.-in-part of U.S. Ser. No. 537,423.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 20020054855	A1	20020509	US 2001-847134	20010502
US 7060247	B2	20060613		
US 6200546	B1	20010313	US 1998-64499	19980422
US 20020176819	A1	20021128	US 2002-122611	20020412
US 6921526	B2	20050726		
WO 2002087631	A1	20021107	WO 2002-US13840	20020430

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002256425 A1 20021111 AU 2002-256425 20020430
 EP 1385556 A1 20040204 EP 2002-725889 20020430

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 20050163710 A1 20050728 US 2004-25636 20041229
 US 7147838 B2 20061212
 US 20060067886 A1 20060330 US 2005-267001 20051104
 US 20070065362 A1 20070322 US 2006-592864 20061103

PRIORITY APPLN. INFO.: US 1997-44049P P 19970422
 US 1998-64499 A3 19980422
 US 2000-537423 A2 20000329
 US 2001-847134 A 20010502
 US 2002-122611 A3 20020412
 WO 2002-US13840 W 20020430
 US 2004-25636 A1 20041229

AB A compound for use as a therapeutic or diagnostic radiopharmaceutical includes a group capable of complexing a medically useful metal attached to a moiety which is capable of binding to a gastrin releasing peptide receptor. A method for treating a subject having a neoplastic disease includes administering to the subject an effective amount of a radiopharmaceutical having a metal chelated with a chelating group attached to a moiety capable of binding to a gastrin releasing peptide receptor expressed on tumor cells with subsequent internalization inside of the cell. A method of forming a therapeutic or diagnostic compound includes reacting a metal synthon with a chelating group covalently linked with a moiety capable of binding a gastrin releasing peptide receptor. Numerous examples are provided of the preparation, properties, gastrin releasing peptide receptor affinity, tumor uptake and biodistribution of DOTA radionuclide complexes conjugated to bombesin(7-14)NH₂ via linkers such as 5-aminovaleric acid and 8-amino-octanoic acid.

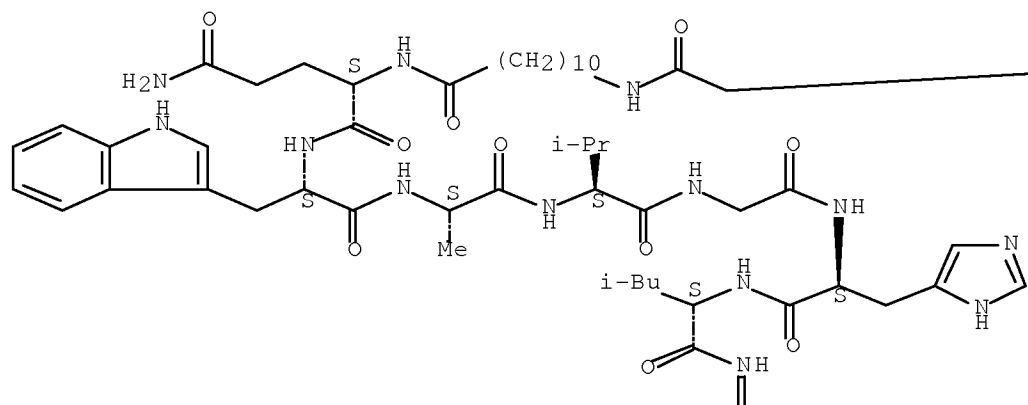
IT 422512-84-3P
 RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (gastrin receptor-avid peptide conjugates and radionuclide complexes: preparation, tumor uptake and biodistribution)

RN 422512-84-3 HCAPLUS

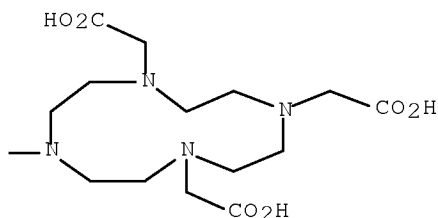
CN L-Methioninamide, N2-[1-oxo-11-[[[4,7,10-tris(carboxymethyl)-1,4,7,10-tetraazacyclododec-1-yl]acetyl]amino]undecyl]-L-glutaminyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

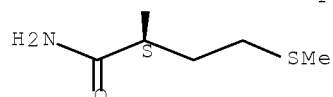
PAGE 1-A



PAGE 1-B



PAGE 2-A



REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:654560 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:347610

ORIGINAL REFERENCE NO.: 129:70673a, 70676a

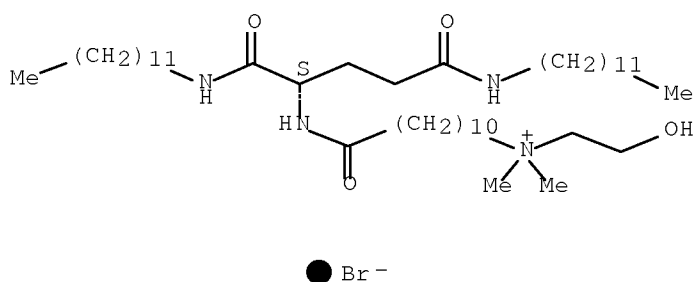
TITLE: AFM observation of organogel nanostructures on graphite in the gel-assisted transfer technique

AUTHOR(S): Kimizuka, Nobuo; Shimizu, Masafumi; Fujikawa, Shigenori; Fujimura, Kotaro; Sano, Masahito; Kunitake, Toyoki

CORPORATE SOURCE: Dep. of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Fukuoka, 812-8581,

	Japan
SOURCE:	Chemistry Letters (1998), (10), 967-968
	CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER:	Chemical Society of Japan
DOCUMENT TYPE:	Journal
LANGUAGE:	English
AB	An ultrathin layer of organogel of L-glutamate-based ammonium amphiphile was transferred from the bulk gel surface onto a graphite plate. Atomic force microscopy showed the presence of fibrous and helical nanostructures on graphite, which existed at the original gel surface.
IT	215612-51-4
	RL: PRP (Properties)
	(fibrous aggregate nanostructure of ammonium L-glutamate amphiphile layer on graphite produced by gel-assisted transfer and observed using AFM)
RN	215612-51-4 HCAPLUS
CN	1-Undecanaminium, 11-[[[(1S)-4-(dodecylamino)-1-[(dodecylamino)carbonyl]-4-oxobutyl]amino]-N-(2-hydroxyethyl)-N,N-dimethyl-11-oxo-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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